

=> file reg
COST IN U.S. DOLLARS SINCE FILE TOTAL
 ENTRY SESSION
FULL ESTIMATED COST 0.21 0.21

FILE 'REGISTRY' ENTERED AT 11:23:38 ON 02 JUN 2008
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

COPYRIGHT (C) 2008 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES: 1 JUN 2008 HIGHEST RN 1024587-16-3
DICTIONARY FILE UPDATES: 1 JUN 2008 HIGHEST RN 1024587-16-3

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 9, 2008.

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10551343\broad.str



```

chain nodes :
7  8  9 10 11 12 13 15 16 17 18
ring nodes :
1  2  3  4  5  6
chain bonds :
1-10  2-11  3-12  4-7  6-9  7-8  8-13  13-15  15-16  16-17  16-18
ring bonds :
1-2  1-6  2-3  3-4  4-5  5-6
exact/norm bonds :
1-2  1-6  1-10  2-3  2-11  3-4  3-12  4-5  5-6  6-9  7-8  8-13  13-15  15-16  16-17
16-18
exact bonds :
4-7

```

G1:O,S

```

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:CLASS 12:CLASS 13:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS

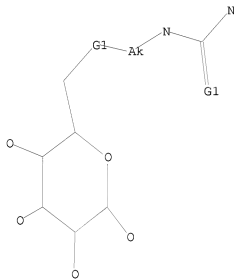
```

L1 STRUCTURE UPLOADED

```

=> d
L1 HAS NO ANSWERS
L1 STR

```



G1 O,S

Structure attributes must be viewed using STN Express query preparation.

```

=> s l1
SAMPLE SEARCH INITIATED 11:23:58 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 174 TO ITERATE

```

100.0% PROCESSED 174 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 2689 TO 4271
PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> s l1 full
FULL SEARCH INITIATED 11:24:03 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 3373 TO ITERATE

100.0% PROCESSED 3373 ITERATIONS 11 ANSWERS
SEARCH TIME: 00.00.01

L3 11 SEA SSS FUL L1

=> file caplus
COST IN U.S. DOLLARS SINCE FILE TOTAL
ENTRY SESSION
FULL ESTIMATED COST 178.36 178.57

FILE 'CAPLUS' ENTERED AT 11:24:07 ON 02 JUN 2008
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2008 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 2 Jun 2008 VOL 148 ISS 23
FILE LAST UPDATED: 1 Jun 2008 (20080601/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

<http://www.cas.org/legal/infopolicy.html>

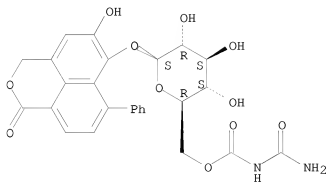
=> s l3
L4 12 L3

=> d l4 1-12 ibib abs hitstr

L4 ANSWER 1 OF 12 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2007:128262 CAPLUS <<LOGINID:20080602>>
DOCUMENT NUMBER: 147:400820
TITLE: Laser microdissection and cryogenic nuclear magnetic resonance spectroscopy: An alliance for cell

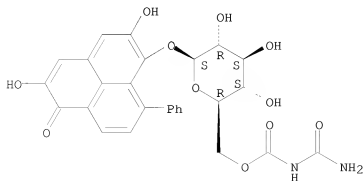
type-specific metabolite profiling. [Erratum to document cited in CA147:380704]
 AUTHOR(S): Hoelscher, D.; Schneider, B.
 CORPORATE SOURCE: Beutenberg Campus, Max-Planck-Institut fuer Chemische Oekologie, Jena, 07745, Germany
 SOURCE: Planta (2007), 225(3), 781
 CODEN: PLANAB; ISSN: 0032-0935
 PUBLISHER: Springer
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB On page 781, the Author line and Affiliation line are incorrect. The correct versions of each are given.
 IT 455255-52-4P 455255-54-6P
 RL: ANT (Analyte); BSU (Biological study, unclassified); PUR (Purification or recovery); ANST (Analytical study); BIOL (Biological study); PREP (Preparation)
 (laser microdissection and cryogenic NMR spectroscopy for plant cell methoxyphenylphenalenones (Erratum))
 RN 455255-52-4 CAPLUS
 CN 1H,3H-Naphtho[1,8-cd]pyran-1-one, 6-[[6-O-[[[(aminocarbonyl)amino]carbonyl]-β-D-glucopyranosyl]oxy]-5-hydroxy-7-phenyl]- (CA INDEX NAME)

Absolute stereochemistry.



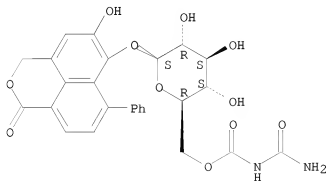
RN 455255-54-6 CAPLUS
 CN 1H-Phenalen-1-one, 6-[[[6-O-[[[(aminocarbonyl)amino]carbonyl]-β-D-glucopyranosyl]oxy]-2,5-dihydroxy-7-phenyl]- (CA INDEX NAME)

Absolute stereochemistry.



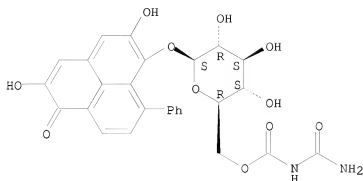
L4 ANSWER 2 OF 12 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2007:128259 CAPLUS <<LOGINID::20080602>>
 DOCUMENT NUMBER: 147:380704
 TITLE: Laser microdissection and cryogenic nuclear magnetic resonance spectroscopy: An alliance for cell type-specific metabolite profiling
 AUTHOR(S): Schneider, B.; Hoelscher, D.
 CORPORATE SOURCE: Beutenberg Campus, Max-Planck-Institut fuer Chemische Oekologie, Jena, 07745, Germany
 SOURCE: Planta (2007), 225(3), 763-770
 CODEN: PLANAB; ISSN: 0032-0935
 PUBLISHER: Springer
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB Laser microdissection was used as a tool to harvest secretory cavities (SC) from leaves of *Dilataris pillansii* Barker (Haemodoraceae) and from leaves and flowers of herbarium specimens of *Dilataris corymbosa* Berg. and *Dilataris viscosa* L. Cryogenic ¹H NMR spectroscopy and HPLC anal. of microdissected samples indicated specific accumulation of methoxyphenylphenalenones in the SC. The structures of two novel and a known natural product in the secretory tissue were confirmed by comparison with authentic comps. isolated from rhizomes and roots from which further phenylphenalenones and phenylphenalenone glucosides were isolated and identified by spectroscopic methods. How it will be possible to use the LMD technique to localize natural products in specific plant cell populations is also discussed.
 IT 455255-52-4P 455255-54-6P
 RL: ANT (Analyte); BSU (Biological study, unclassified); PUR (Purification or recovery); ANST (Analytical study); BIOL (Biological study); PREP (Preparation)
 (laser microdissection and cryogenic NMR spectroscopy for plant cell methoxyphenylphenalenones)
 RN 455255-52-4 CAPLUS
 CN 1H,3H-Naphtho[1,8-cd]pyran-1-one, 6-[[6-O-[[{(aminocarbonyl)amino}carbonyl]-β-D-glucopyranosyl]oxy]-5-hydroxy-7-phenyl]- (CA INDEX NAME)

Absolute stereochemistry.



RN 455255-54-6 CAPLUS
 CN 1H-Phenalen-1-one, 6-[[6-O-[[{(aminocarbonyl)amino}carbonyl]-β-D-glucopyranosyl]oxy]-2,5-dihydroxy-7-phenyl]- (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 12 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2006:615923 CAPLUS <<LOGINID:20080602>>

DOCUMENT NUMBER: 146:157982

TITLE: A type III polyketide synthase from *Wachendorfia thyrsiflora* and its role in diarylheptanoid and phenylphenalenone biosynthesis

AUTHOR(S): Brand, S.; Hoelscher, D.; Schierhorn, A.; Svatos, A.; Schroeder, J.; Schneider, B.

CORPORATE SOURCE: Max-Planck-Institut fuer Chemische Oekologie, Beutenberg Campus, Jena, 07745, Germany

SOURCE: Planta (2006), 224(2), 413-428
CODEN: PLANAB; ISSN: 0032-0935

PUBLISHER: Springer

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Chalcone synthase (CHS) related type III plant polyketide synthases (PKSs) are likely to be involved in the biosynthesis of diarylheptanoids (e.g. curcumin and polycyclic phenylphenalenones), but no such activity has been reported. Root cultures from *Wachendorfia thyrsiflora* (Haemodoraceae) are a suitable source to search for such enzymes because they synthesize large amounts of phenylphenalenones, but no other products that are known to require CHSs or related enzymes (e.g. flavonoids or stilbenes). A homol.-based RT-PCR strategy led to the identification of cDNAs for a type III PKS sharing only approx. 60% identity with typical CHSs. It was named WtPKS1 (*W. thyrsiflora* polyketide synthase 1). The purified recombinant protein accepted a large variety of aromatic and aliphatic starter CoA esters, including phenylpropionyl- and side-chain unsatd. phenylpropanoid-CoAs. The simplest model for the initial reaction in diarylheptanoid biosynthesis predicts a phenylpropanoid-CoA as starter and a single condensation reaction to a diketide. Benzalacetones, the expected release products, were observed only with unsatd. phenylpropanoid-CoAs, and the best results were obtained with 4-coumaroyl-CoA (80% of the products). With all other substrates, WtPKS1 performed two condensation reactions and released pyrones. We propose that WtPKS1 catalyzes the first step in diarylheptanoid biosynthesis and that the observed pyrones are derailment products in the absence of downstream processing proteins.

IT 455255-52-4 455255-54-6

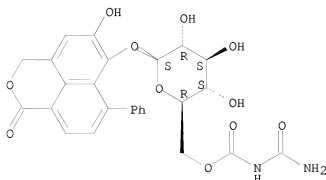
RL: BSU (Biological study, unclassified); NPO (Natural product occurrence); BIOL (Biological study); OCCU (Occurrence)

(type III polyketide synthase from *Wachendorfia thyrsiflora* and its role in diarylheptanoid and phenylphenalenone biosynthesis)

RN 455255-52-4 CAPLUS

CN 1H,3H-Naphtho[1,8-cd]pyran-1-one, 6-[[6-O-[(aminocarbonyl)amino]carbonyl]- β -D-glucopyranosyl]oxy]-5-hydroxy-7-phenyl- (CA INDEX NAME)

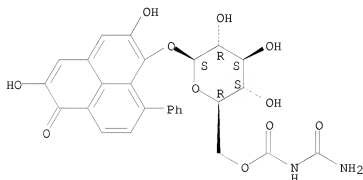
Absolute stereochemistry.



RN 455255-54-6 CAPLUS

CN 1H-Phenalen-1-one, 6-[[6-O-[(aminocarbonyl)amino]carbonyl]- β -D-glucopyranosyl]oxy]-2,5-dihydroxy-7-phenyl- (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 46 THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 4 OF 12 CAPLUS COPYRIGHT 2008 ACS ON STN

ACCESSION NUMBER: 2005:889890 CAPLUS <<LOGINID:20080602>>

DOCUMENT NUMBER: 143:362725

TITLE: HPLC-NMR for tissue-specific analysis of phenylphenalenone-related compounds in *Xiphidium caeruleum* (Haemodoraceae)

AUTHOR(S): Schneider, Bernd; Paetz, Christian; Hoelscher, Dirk; Opitz, Stefan

CORPORATE SOURCE: Max-Planck-Institute for Chemical Ecology, Jena, 07745, Germany

SOURCE: Magnetic Resonance in Chemistry (2005), 43(9), 724-728
CODEN: MRCHEG; ISSN: 0749-1581

PUBLISHER: John Wiley & Sons Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB HPLC-1H NMR has been used to study the tissue-specific distribution of phenylphenalenones, polyphenolic natural products of *Xiphidium caeruleum*, a neotropical member of the Haemodoraceae plant family. The present results provide insight into the occurrence of phenylphenalenone-related compds. in root segments of whole plants and different in vitro culture lines of the same species.

IT 455255-54-6

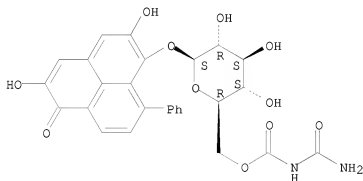
RL: ANT (Analyte); BSU (Biological study, unclassified); NPO (Natural product occurrence); ANST (Analytical study); BIOL (Biological study); OCCU (Occurrence)

(HPLC-NMR for tissue-specific anal. of phenylphenalenone-related compds. in *Xiphidium caeruleum* (Haemodoraceae))

RN 455255-54-6 CAPLUS

CN 1H-Phenalen-1-one, 6-[[6-O-[(aminocarbonyl)amino]carbonyl]- β -D-glucopyranosyl]oxy]-2,5-dihydroxy-7-phenyl- (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 5 OF 12 CAPLUS COPYRIGHT 2008 ACS ON STN

ACCESSION NUMBER: 2004:495129 CAPLUS <<LOGINID:20080602>>

DOCUMENT NUMBER: 142:56578

TITLE: Functional evaluation of carbohydrate-centered glycoclusters by enzyme-linked lectin assay: Ligands for concanavalin A

AUTHOR(S): Koehn, Maja; Benito, Juan M.; Mellet, Carmen Ortiz; Lindhorst, Thisbe K.; Fernandez, Jose M. Garcia

CORPORATE SOURCE: Instituto de Investigaciones Químicas, CSIC, Seville, 41092, Spain

SOURCE: ChemBioChem (2004), 5(6), 771-777

CODEN: CBCHFX; ISSN: 1439-4227

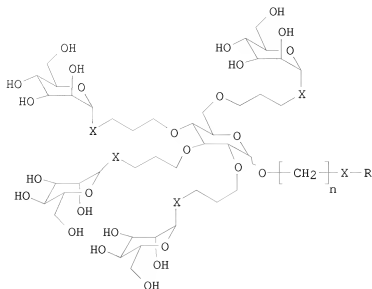
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 142:56578

GI



I

AB The affinities of the mannose-specific lectin Con A towards D-glucose-centered mannosyl clusters differing in the anomeric configuration of the monosaccharide core, nature of the bridging functional groups and valency, have been measured by a competitive enzyme-linked lectin assay. Pentavalent thioether-linked ligands I ($X = S, n = 3, R = \alpha\text{-D-mannopyranosyl}$) were prepared by radical addition of 2,3,4,6-tetra-O-acetyl-1-thio- $\alpha\text{-D-mannopyranose}$ to the corresponding penta-O-allyl- α - or - $\beta\text{-D-glucopyranose}$, followed by deacetylation. The distinct reactivity of the anomeric position in the D-glucose scaffold was exploited in the preparation of a tetravalent cluster I ($X = S, n = 6, R = \text{Br}$) (II) that keeps a reactive aglyconic group for further manipulation, including incorporation of a reporter group or attachment to a solid support. Hydroboration of the double bonds in the penta-O-allyl- $\alpha\text{-D-glucopyranose}$ derivative and replacement of the hydroxy groups with amine moieties gave a suitable precursor for the preparation of pentavalent and 15-valent mannosides through the thiourea-bridging reaction I ($X = \text{NHC(S)NH}, n = 3, R = \alpha\text{-D-mannopyranosyl}$) (III). The diastereomeric 1-thiomannose-coated clusters I were demonstrated to be potent ligands for Con A, with IC50 values for the inhibition of the Con A-yeast mannan association indicative of 6.4- and 5.5-fold increases in binding affinity (valency-corrected values), resp., relative to the value for Me $\alpha\text{-D-mannopyranoside}$. The tetravalent cluster II exhibited a valency-corrected relative lectin-binding potency virtually identical to that of the homologous pentavalent mannoside. In sharp contrast, replacement of the 1-thiomannose wedges of I with $\alpha\text{-D-mannopyranosylthioureido}$ units III virtually abolished any multivalent or statistic effects, with a dramatic decrease of binding affinity. The 15-valent ligand possessing classical O-glycosidic linkages, exhibited a two-fold increase in lectin affinity relative to the penta-O-(thioglycoside); it is less efficient based on the number of mannose units. The results illustrate the potential of carbohydrates as polyfunctional platforms for glycocluster construction and underline the importance of careful design of the overall architecture in optimizing glycocluster recognition by specific lectins.

IT 808137-83-9P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL

(Biological study); PREP (Preparation)

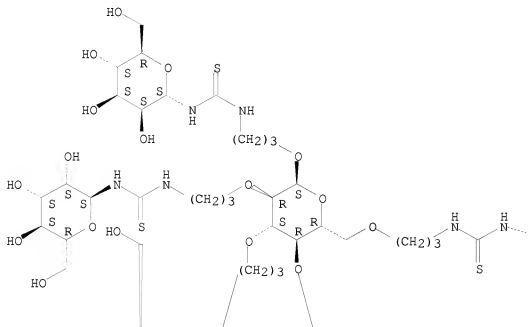
(preparation and evaluation of glucose-centered mannosyl glycoclusters by enzyme-linked lectin assay as ligand to Con A)

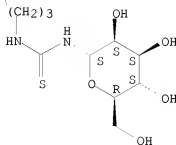
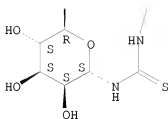
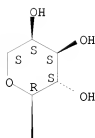
RN 808137-83-9 CAPLUS

CN Thiourea, N- α -D-mannopyranosyl-N'-[3-[[2,3,4,6-tetrakis-O-[3-[[α -D-mannopyranosylamino)thioxomethylamino]propyl]- α -D-glucopyranosyl]oxy]propyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

PAGE 1-A





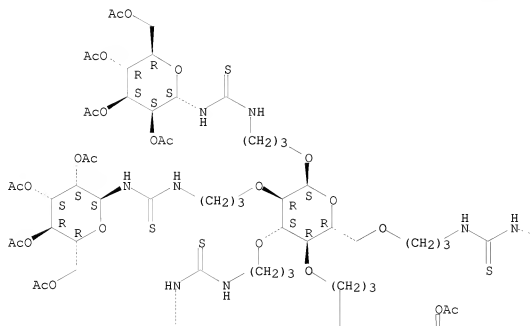
IT 808137-82-8P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (preparation and evaluation of glucose-centered mannosyl glycoclusters by
 enzyme-linked lectin assay as ligand to Con A)

RN 808137-82-8 CAPLUS

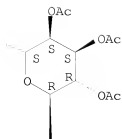
CN Thiourea, N-(2,3,4,6-tetra-O-acetyl- α -D-mannopyranosyl)-N'-[3-
[[2,3,4,6-tetrakis-O-[3-[[[(2,3,4,6-tetra-O-acetyl- α -D-
mannopyranosyl)amino]thioxomethyl]amino]propyl]- α -D-
glucopyranosyl]oxylpropyl]- (9CI) (CA INDEX NAME)

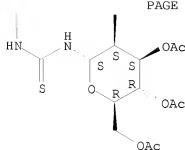
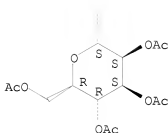
Absolute stereochemistry. Rotation (+).

PAGE 1-A



PAGE 1-B





PAGE 2-A



PAGE 2-B

REFERENCE COUNT: 60 THERE ARE 60 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 6 OF 12 CAPLUS COPYRIGHT 2008 ACS ON STN
 ACCESSION NUMBER: 2003:290736 CAPLUS <<LOGINID:20080602>>
 DOCUMENT NUMBER: 139:162042
 TITLE: Histochemical analysis of phenylphenalenone-related compounds in Xiphidium caeruleum (haemodoraceae)
 AUTHOR(S): Opitz, S.; Schnitzler, J.-P.; Hause, B.; Schneider, B.
 CORPORATE SOURCE: Max-Planck-Institute for Chemical Ecology, Jena, 07745, Germany
 SOURCE: Planta (2003), 216(5), 881-889
 CODEN: PLANAB; ISSN: 0032-0935
 PUBLISHER: Springer-Verlag
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB Phenylphenalenones represent a typical group of secondary metabolites of the Haemodoraceae. Some of these phenolic compds. show organ-specific distribution within the plant. However, detailed information on cellular localization is still lacking. To this end, confocal laser-scanning microscopy, microspectral photometry and high-performance liquid chromatog. were used to study the tissue localization of phenylphenalenone-type compds. in Xiphidium caeruleum Aubl. From the autofluorescence potential of these compds., specific distribution of allophanylglucosides and non-glucosidic compds. of the phenylphenalenone-type in distinct cells of the roots (apical meristem, cortex, cap, epidermis) and the shoot system was revealed. Fluorescence enhancement using "Naturstoff reagent A" (NA) indicated the occurrence of NA-pos. natural products in the vacuoles of leaf epidermal cells. The present results provide new insights into the possible functions of phenylphenalenone-related compds. in the context of their localization. Addnl., the advantages and limitations of the techniques are discussed.

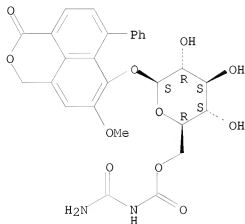
IT 455255-53-5 455255-55-7

RL: BSU (Biological study, unclassified); BIOL (Biological study)
(histochem. anal. of phenylphenalenone-related compds. in *Xiphidium caeruleum*)

RN 455255-53-5 CAPLUS

CN 1H,3H-Naphtho[1,8-cd]pyran-1-one, 6-[[6-O-[[[(aminocarbonyl)amino]carbonyl]- β -D-glucopyranosyl]oxy]-5-methoxy-7-phenyl- (CA INDEX NAME)

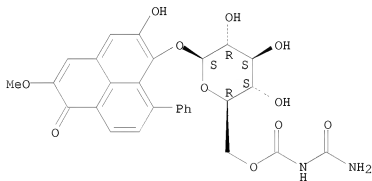
Absolute stereochemistry.



RN 455255-55-7 CAPLUS

CN 1H-Phenalen-1-one, 6-[[6-O-[[[(aminocarbonyl)amino]carbonyl]- β -D-glucopyranosyl]oxy]-5-hydroxy-2-methoxy-7-phenyl- (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 7 OF 12 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2003:161564 CAPLUS <<LOGINID:20080602>>

DOCUMENT NUMBER: 139:19580

TITLE: Oxidative biosynthesis of phenylbenzoisochromenones from phenylphenalenones

AUTHOR(S): Opitz, Stefan; Schneider, Bernd

CORPORATE SOURCE: Max-Planck-Institut fuer Chemische Okologie, Jena, D-07745, Germany

SOURCE: Phytochemistry (Elsevier) (2003), 62(3), 307-312
 CODEN: PYTCAS; ISSN: 0031-9422
 PUBLISHER: Elsevier Science Ltd.
 DOCUMENT TYPE: Journal
 LANGUAGE: English

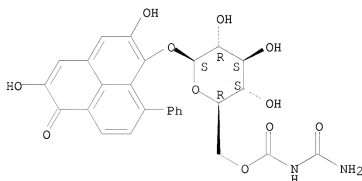
AB 13C NMR anal. demonstrated incorporation of two 13C labeled phenylalanine units into phenylphenalenones and phenylbenzoisochromenones co-occurring in *Wachendorfia thyrsiflora*. These results suggest oxidative formation of phenylbenzoisochromenones following a late branching from a common phenylphenalenone biosynthetic pathway. A dioxygenase-type mechanism, followed by decarboxylation, is suggested for the key steps of this conversion.

IT 455255-54-6
 RL: BSU (Biological study, unclassified); BIOL (Biological study) (oxidative biosynthesis of phenylbenzoisochromenones from phenylphenalenones)

RN 455255-54-6 CAPLUS

CN 1H-Phenalen-1-one, 6-[[6-O-[[[(aminocarbonyl)amino]carbonyl]-β-D-glucopyranosyl]oxy]-2,5-dihydroxy-7-phenyl- (CA INDEX NAME)

Absolute stereochemistry.

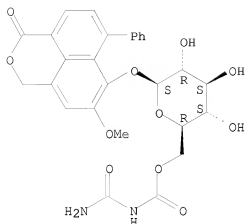


IT 455255-53-5
 RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study) (oxidative biosynthesis of phenylbenzoisochromenones from phenylphenalenones)

RN 455255-53-5 CAPLUS

CN 1H,3H-Naphtho[1,8-cd]pyran-1-one, 6-[[6-O-[[[(aminocarbonyl)amino]carbonyl]-β-D-glucopyranosyl]oxy]-5-methoxy-7-phenyl- (CA INDEX NAME)

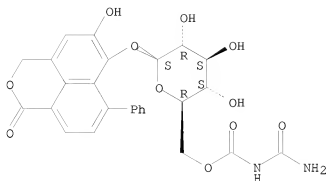
Absolute stereochemistry.



REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 8 OF 12 CAPLUS COPYRIGHT 2008 ACS ON STN
 ACCESSION NUMBER: 2002:895377 CAPLUS <<LOGINID::20080602>>
 DOCUMENT NUMBER: 139:66030
 TITLE: Organ-specific analysis of phenylphenalenone-related compounds in *Xiphidium caeruleum*
 AUTHOR(S): Opitz, Stefan; Schneider, Bernd
 CORPORATE SOURCE: Max-Planck-Institut für Chemische Ökologie, Jena, D-07745, Germany
 SOURCE: Phytochemistry (Elsevier) (2002), 61(7), 819-825
 CODEN: PYTCAS; ISSN: 0031-9422
 PUBLISHER: Elsevier Science Ltd.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB The distribution pattern of phenylphenalenone-type compds. was investigated in vegetative and reproductive organs of *Xiphidium caeruleum*. The highest total molar concentration, up to 30 $\mu\text{mol g}^{-1}$ fr. wt, was detected in the root tip and the stamen. Accumulation of specific phenylphenalenone-related metabolites including glycosides was found in the hypogaeal plant parts, the leaves, and the reproductive organs of the inflorescence. Putative biosynthetic relationships and the role of these compds. in plant defense are discussed.
 IT 455255-52-4P 455255-53-5P 455255-54-6P
455255-55-7P
 RL: BSU (Biological study, unclassified); PUR (Purification or recovery); BIOL (Biological study); PREP (Preparation)
 (phenylphenalenone-related compds. in *Xiphidium caeruleum*)
 RN 455255-52-4 CAPLUS
 CN 1H,3H-Naphtho[1,8-cd]pyran-1-one, 6-[[6-O-[[[(aminocarbonyl)amino]carbonyl]- β -D-glucopyranosyl]oxy]-5-hydroxy-7-phenyl- (CA INDEX NAME)

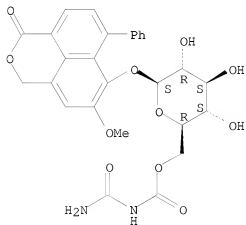
Absolute stereochemistry.



RN 455255-53-5 CAPLUS

CN 1H,3H-Naphtho[1,8-cd]pyran-1-one, 6-[[6-O-[[[(aminocarbonyl)amino]carbonyl]-β-D-glucopyranosyl]oxy]-5-methoxy-7-phenyl- (CA INDEX NAME)

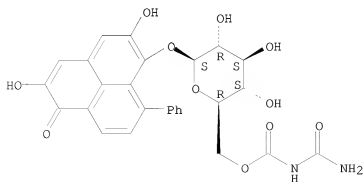
Absolute stereochemistry.



RN 455255-54-6 CAPLUS

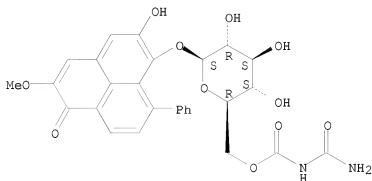
CN 1H-Phenalen-1-one, 6-[[6-O-[[[(aminocarbonyl)amino]carbonyl]-β-D-glucopyranosyl]oxy]-2,5-dihydroxy-7-phenyl- (CA INDEX NAME)

Absolute stereochemistry.



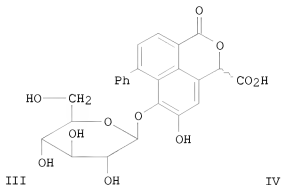
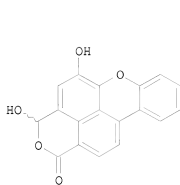
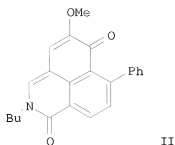
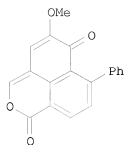
RN 455255-55-7 CAPLUS
CN 1H-Phenalen-1-one, 6-[[6-O-[[[(aminocarbonyl)amino]carbonyl]-β-D-glucopyranosyl]oxy]-5-hydroxy-2-methoxy-7-phenyl- (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 9 OF 12 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2002:515160 CAPLUS <<LOGINID:20080602>>
DOCUMENT NUMBER: 137:213636
TITLE: Phenylphenalenone-related compounds: Chemotaxonomic markers of the Haemodoraceae from *Xiphidium caeruleum*
AUTHOR(S): Opitz, Stefan; Hoelscher, Dirk; Oldham, Neil J.; Bartram, Stefan; Schneider, Bernd
CORPORATE SOURCE: Max Planck Institute for Chemical Ecology, Jena, 07745, Germany
SOURCE: Journal of Natural Products (2002), 65(8), 1122-1130
CODEN: JNPRDF; ISSN: 0163-3864
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



AB Phytochem. anal. of *Xiphidium caeruleum*, a neotropical member of the family Haemodoraceae, resulted in the isolation and identification of a variety of phenylphenalenone-related compds. The structures of four new phenylbenzoisochromenones (e.g. I), a new phenylbenzoisoquinolinone (II), and two new oxabenzochrysenones (e.g. III) were elucidated using MS and NMR spectroscopic techniques. In addition, five new glucosides (e.g. IV) were identified, among them four allophanyl glucosides, representing a novel type of 6'-substituted glucosidic natural product. On the basis of the common occurrence of these 12 new and four known structures, hypothetical biosynthetic relationships are discussed. The natural product distribution of other genera of the Haemodoraceae is used as the basis to elaborate biogeog. characteristics of this plant family.

IT 455255-52-4P 455255-53-5P 455255-54-6P
455255-55-7P

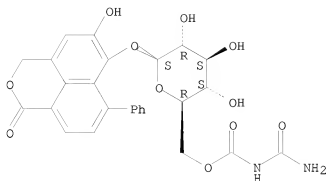
RL: NPO (Natural product occurrence); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)

(phenylphenalenone-related compds. from *Xiphidium caeruleum*)

RN 455255-52-4 CAPLUS

CN 1H,3H-Naphtho[1,8-cd]pyran-1-one, 6-[[6-O-[[[(aminocarbonyl)amino]carbonyl]- β -D-glucopyranosyl]oxy]-5-hydroxy-7-phenyl]- (CA INDEX NAME)

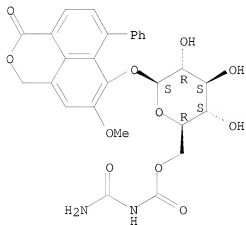
Absolute stereochemistry.



RN 455255-53-5 CAPLUS

CN 1H,3H-Naphtho[1,8-cd]pyran-1-one, 6-[[6-O-[[[(aminocarbonyl)amino]carbonyl]-β-D-glucopyranosyl]oxy]-5-methoxy-7-phenyl- (CA INDEX NAME)

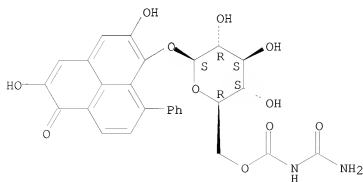
Absolute stereochemistry.



RN 455255-54-6 CAPLUS

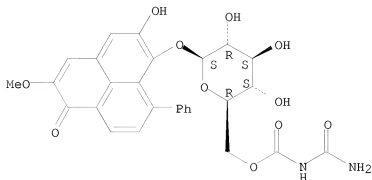
CN 1H-Phenalen-1-one, 6-[[6-O-[[[(aminocarbonyl)amino]carbonyl]-β-D-glucopyranosyl]oxy]-2,5-dihydroxy-7-phenyl- (CA INDEX NAME)

Absolute stereochemistry.



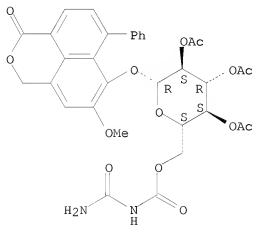
RN 455255-55-7 CAPLUS
 CN 1H-Phenalen-1-one, 6-[[6-O-[[[(aminocarbonyl)amino]carbonyl]- β -D-glucopyranosyl]oxy]-5-hydroxy-2-methoxy-7-phenyl- (CA INDEX NAME)

Absolute stereochemistry.



IT 455255-57-9
 RL: PRP (Properties)
 (properties of)
 RN 455255-57-9 CAPLUS
 CN 1H,3H-Naphtho[1,8-cd]pyran-1-one, 5-methoxy-7-phenyl-6-[[2,3,4-tri-O-acetyl-6-O-[[[(aminocarbonyl)amino]carbonyl]- β -D-glucopyranosyl]oxy]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 10 OF 12 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2001:823666 CAPLUS <<LOGINID:20080602>>
 DOCUMENT NUMBER: 136:86015
 TITLE: Trehalose-Based Octopus Glycosides for the Synthesis of Carbohydrate-Centered PAMAM Dendrimers and Thiourea-Bridged Glycoclusters

AUTHOR(S): Dubber, Michael; Lindhorst, Thisbe K.
 CORPORATE SOURCE: Institut fuer Organische Chemie, Christian-Albrechts-
 Universitaet zu Kiel, Kiel, D-24098, Germany
 SOURCE: Organic Letters (2001), 3(25), 4019-4022
 CODEN: ORLEF7; ISSN: 1523-7060
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 136:86015

AB The nonreducing disaccharide trehalose was modified into an octa-amino-functionalized core mol. to serve in the synthesis of carbohydrate-centered PAMAM glycodendrimers and thiourea-bridged glycoclusters.

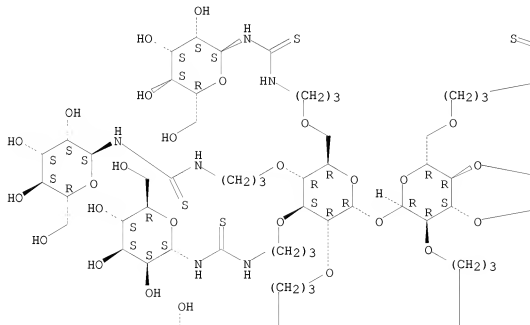
IT 386264-10-4P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (trehalose-based octopus glycosides for the synthesis of carbohydrate-centered PAMAM dendrimers and thiourea-bridged glycoclusters)

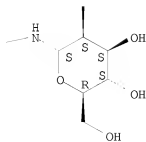
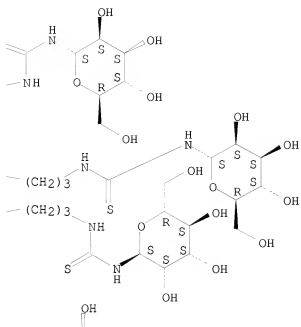
RN 386264-10-4 CAPLUS

CN α -D-Glucopyranoside, 2,3,4,6-tetrakis-O-[3-[[α -D-mannopyranosylamino)thioxomethyl]amino]propyl]- α -D-glucopyranosyl 2,3,4,6-tetrakis-O-[3-[[α -D-mannopyranosylamino)thioxomethyl]amino]propyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

PAGE 1-A

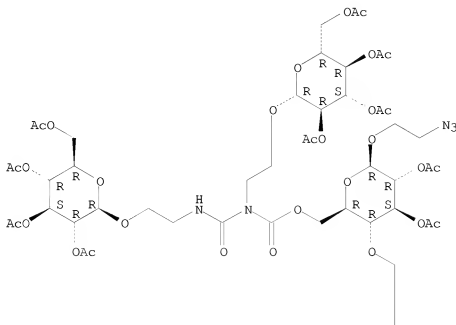




L4 ANSWER 11 OF 12 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2000:396983 CAPLUS <<LOGINID::20080602>>
 DOCUMENT NUMBER: 133:193346
 TITLE: Synthesis of Allophanate-Derived Branched Glycoforms from Alcohols and p-Nitrophenyl Carbamates
 AUTHOR(S): Chong, Pek Y.; Petillo, Peter A.
 CORPORATE SOURCE: Department of Chemistry, University of Illinois at Urbana-Champaign, Urbana, IL, 61801, USA
 SOURCE: Organic Letters (2000), 2(14), 2113-2116
 CODEN: ORLEF7; ISSN: 1523-7060
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 133:193346
 AB The formation of saccharide-derived carbamates and alkyl 2,4-dialkylallophanates from alcs. and p-nitrophenyl carbamates was described. Optimization of allophanate formation led to the synthesis of branched glycoforms with inter-saccharide allophanate linkages that are rigidified by intramol. hydrogen bonds.
 IT 288844-61-1P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (synthesis of allophanate-derived branched glycoforms from alcs. and p-nitrophenyl carbamates)
 RN 288844-61-1 CAPLUS
 CN β -D-Glucopyranoside, 2-azidoethyl 4-O-[(4-methoxyphenyl)methyl]-, 2,3-diacetate 6-[[2-[(2,3,4,6-tetra-O-acetyl- β -D-glucopyranosyl)oxy]ethyl][[2-[(2,3,4,6-tetra-O-acetyl- β -D-glucopyranosyl)oxy]ethyl]amino]carbonyl]carbamate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A





REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 12 OF 12 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2000:314834 CAPLUS <<LOGINID::20080602>>
 DOCUMENT NUMBER: 132:344104
 TITLE: Cloning and production of human adenine nucleotide translocator and the synthesis and screening assays for novel ligands
 INVENTOR(S): Anderson, Christen M.; Davis, Robert E.; Clevenger, William; Wiley, Sandra Eileen; Miller, Scott W.; Szabo, Tomas R.; Ghosh, Soumitra S.
 PATENT ASSIGNEE(S): Mitokor, USA
 SOURCE: PCT Int. Appl., 175 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 2
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000026370	A2	20000511	WO 1999-US25883	19991103
WO 2000026370	A3	20001116		
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
US 6906173	B2	20050614	US 1998-185904	19981103
US 2002177185	A1	20050614		
CA 2349444	A1	20000511	CA 1999-2349444	19991103
AU 2000024729	A	20000522	AU 2000-24729	19991103
AU 769756	B2	20040205		
EP 1049780	A1	20001108	EP 1999-968032	19991103
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
JP 2002539761	T	20021126	JP 2000-579742	19991103
US 20010044144	A1	20011122	US 2001-811094	20010314
US 6902908	B2	20050607		
US 20020012992	A1	20020131	US 2001-810644	20010314
US 20050019835	A1	20050127	US 2001-811131	20010314
US 7001729	B2	20060221		
US 20050064530	A1	20050324	US 2001-811132	20010314

US 6887670	B2	20050503		
US 20050003352	A1	20050106	US 2001-809827	20010316
US 6906174	B2	20050614		
US 20050003353	A1	20050106	US 2001-809889	20010316
US 6906175	B2	20050614		
AU 2002029270	A	20020523	AU 2002-29270	20020328
AU 782387	B2	20050721		
AU 2002029293	A	20020523	AU 2002-29293	20020328
AU 782476	B2	20050804		
AU 2002029295	A	20020523	AU 2002-29295	20020328
AU 782449	B2	20050728		
JP 2004154139	A	20040603	JP 2003-408115	20031205
US 20040241801	A1	20041202	US 2004-763398	20040123
PRIORITY APPLN. INFO.:			US 1998-185904	A 19981103
			US 1999-393441	A 19990908
			AU 2000-24729	A3 19991103
			JP 2000-579742	A3 19991103
			WO 1999-US25883	W 19991103
			US 2000-569327	B1 20000511

OTHER SOURCE(S): MARPAT 132:344104

AB Compns. and methods are provided for producing adenine nucleotide translocator (ANT) polypeptides and fusion proteins, including the production and use of recombinant expression constructs having a regulated promoter. Bacterial, insect, yeast (Sf9 cells and Trichoplusia ni cells), and mammalian expression systems are designed for reliable production of recombinant human ANT polypeptides in significant quantities, by employing regulated promoters and recombinant ANT fusion products with glutathione S-transferase and green fluorescent protein. The synthesis and properties of representative atractyloside derivs. as ANT ligands are described. ANT ligands and compns. and methods for identifying ANT ligands, agents that bind ANT, and agents that interact with ANT are also disclosed.

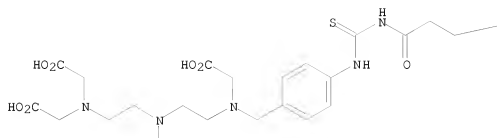
IT 267886-22-6P 267886-30-6P
 RL: ARG (Analytical reagent use); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); USES (Uses)
 (cloning and production of human adenine nucleotide translocator and the synthesis and screening assays for novel ligands)

RN 267886-22-6 CAPLUS

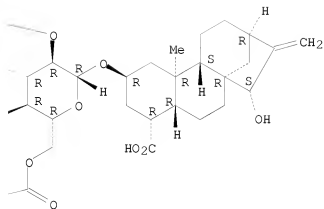
CN 19-Norkaur-16-en-18-oic acid, 2-[[6-O-[4-[[[4-[[[2-[[2-[bis(carboxymethyl)amino]ethyl](carboxymethyl)amino]ethyl](carboxymethyl)amino]methyl]phenyl]amino]thioxomethyl]amino]-1,4-dioxobutyl]-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo-β-D-glucopyranosyl]oxy]-15-hydroxy-, (2β,4α,15α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



PAGE 2-A



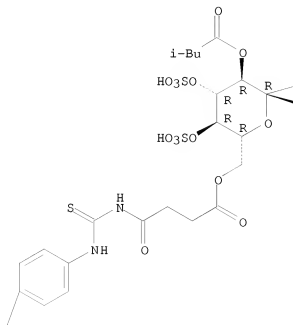
RN 267886-30-6 CAPLUS

CN 19-Norkaur-16-en-18-oic acid, 2-[[[6-O-[4-[[[4-[2-[2,6-bis[3-carboxy-2-(carboxymethyl)propyl]-4-pyridinyl]ethyl]phenyl]amino]thioxomethyl]amino]-

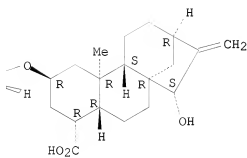
1,4-dioxobutyl]-2-O-(3-methyl-1-oxobutyl)-3,4-di-O-sulfo- β -D-glucopyranosyl]oxy]-15-hydroxy-, (2 β ,4 α ,15 α)- (9CI) (CA INDEX NAME)

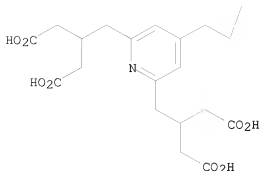
Absolute stereochemistry.

PAGE 1-A



PAGE 1-B





=> file stng

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION

FULL ESTIMATED COST

65.88	244.45
-------	--------

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION

CA SUBSCRIBER PRICE

-9.60	-9.60
-------	-------

FILE 'STNGUIDE' ENTERED AT 11:24:35 ON 02 JUN 2008

USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT

COPYRIGHT (C) 2008 AMERICAN CHEMICAL SOCIETY (ACS)

FILE CONTAINS CURRENT INFORMATION.

LAST RELOADED: May 30, 2008 (20080530/UP).

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION

FULL ESTIMATED COST

0.06	244.51
------	--------

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION

CA SUBSCRIBER PRICE

0.00	-9.60
------	-------

FILE 'CAPLUS' ENTERED AT 11:25:24 ON 02 JUN 2008

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

COPYRIGHT (C) 2008 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE LAST UPDATED: 1 Jun 2008 (20080601/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply.
They are available for your review at:

<http://www.cas.org/legal/infopolicy.html>

```
=> cyclodextrin and thiourea
    36900 CYCLODEXTRIN
    10611 CYCLODEXTRINS
    37912 CYCLODEXTRIN
          (CYCLODEXTRIN OR CYCLODEXTRINS)
    45097 THIOUREA
    5115  THIOUREAS
    46885 THIOUREA
          (THIOUREA OR THIOUREAS)
L5      140 CYCLODEXTRIN AND THIOUREA
```

```
=> 15 and solub?
    278276 SOLUB?
    675932 SOL
    18532  SOLS
    683513 SOL
          (SOL OR SOLS)
    233022 SOLY
    1      SOLIES
    233022 SOLY
          (SOLY OR SOLIES)
    1002403 SOLUB?
          (SOLUB? OR SOL OR SOLY)
L6      29  L5 AND SOLUB?
```

```
=> s 15 and py<=2003
    23980590 PY<=2003
L7      88  L5 AND PY<=2003
```